The Emerging Problem of Novel Psychoactive Substances

In the past few years the world has experienced a large increase in the number of compounds appearing on the illicit drug market. Such substances are designed to circumvent governmental regulations—the manufacturers routinely take a known psychoactive compound reported in the scientific literature and alter it chemically in order to produce compounds that will mimic its pharmacological activity but not have an identical structure to the parent molecule. Many of these substances are sold via the internet or in "head shops". In particular, products known as "bath salts" usually contain mixtures of cathinone-derived compounds with effects such as an increase of the synaptic concentration of biogenic amines (norepinephrine, dopamine, and serotonin).

Another class of potentially dangerous products are sold as "Spice" or "herbal incense" and usually contain mixtures of compounds termed "synthetic cannabinoids" (CB receptor ligands) sprayed onto botanical material. The number of new drugs of abuse appearing on the market is rapidly increasing, making it very difficult for government agencies to control them. Users are attracted by the low cost of these substances. Use and abuse of these products has often been linked to a series of side effects including psychosis, seizures and other psychotropic effects, and in certain cases suicide or death.

The objective of this project is to critically review the present status of NPS, with special regards to structure-activity relationships, synthetic and analytical aspects, and their potential biological effects. The results of this project will aid in educating scientific, social and government bodies with respect to this ever-growing phenomenon and the challenges it poses.

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www.iupac.org/project/2014-019-1-700

Nomenclature of Carbon Nanotubes and Related Substances

The objective of this new project supported by the Chemical Nomenclature and Structure Representation Division (IUPAC Div VIII) is to analyze existing nomenclature principles for carbon nanotubes (CNT) and related substances, and to create a technical report on nomenclature conventions to be used by scientists and regulatory bodies.

Nanomaterials are already a very important area of chemistry with a quickly growing range of industrial applications. IUPAC nomenclature conventions in this area are needed for both scientists and regulatory agencies.

The current IUPAC recommendations in the area of nanomaterials are limited to fullerenes only. Practically all other classes of nanomaterials are as yet out of the scope of IUPAC attention. This project is aimed at the analysis of currently scattered nomenclature conventions for CNT and the preparation of a technical report on nomenclature conventions for classification and naming of CNT and related substances.

Because of the special nature of CNT, the project team is composed of CNT experts and experts in the nomenclature of discrete and macromolecular structures. The involved CNT experts took part in the task group of the Terminology and Nomenclature Working Group of the International Organization for Standardization (ISO) (ISO/TC229 Nanotechnologies).

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Terminology for Modeling and Simulation of Polymers

With ubiquitous access to high performance computing, modeling and simulation have become everyday practices supporting more traditional theoretical approaches to developing our understanding of polymers and their properties. Indeed, the prediction of properties and behaviors of materials well before synthesizing molecular systems is a Holy Grail of modern science. While this holds for all areas of chemistry, the role of simulation and modeling in polymers is particularly significant due to the inherent complexity of even "pure" polymer materials. The nearly infinite possibilities to modulate the structure of polymer molecules often make statistical and modeling approaches mandatory, even to gain a rough interpretation of experimental data.

Difficulties developing sound and detailed structural models stem from the extremely broad range of time- and length-scales of polymeric materials, the possible presence of "morphological constraints"